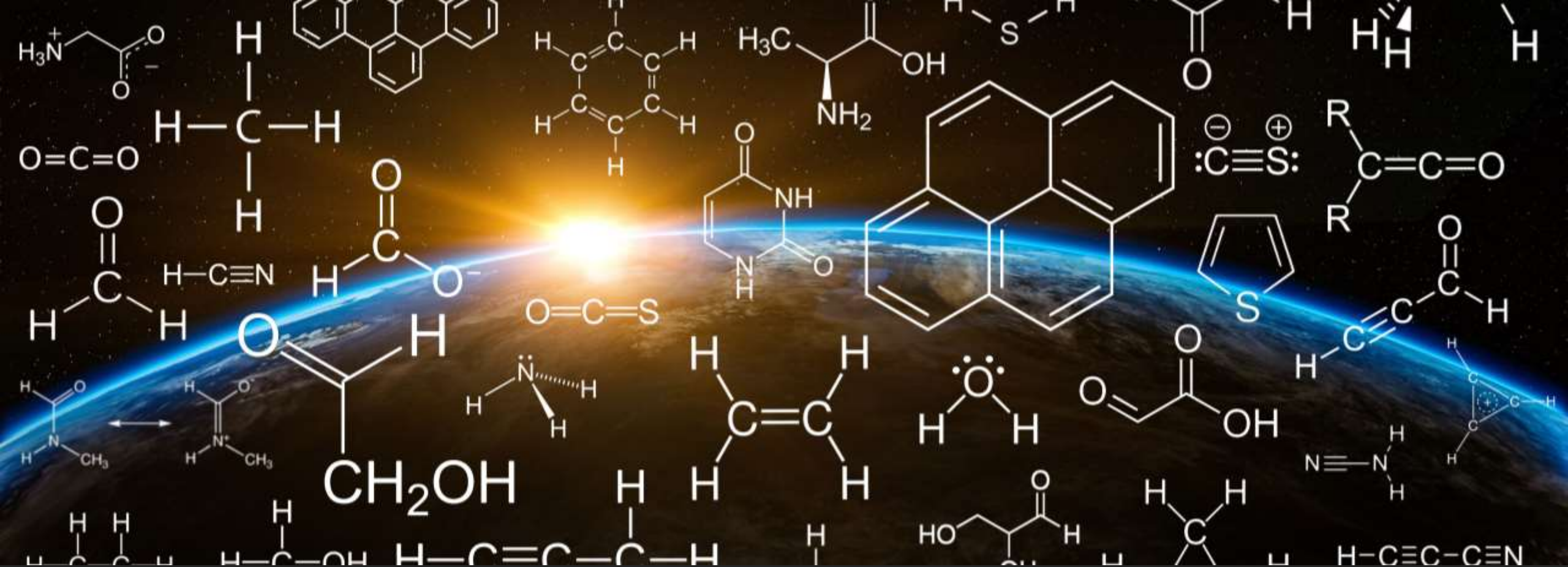
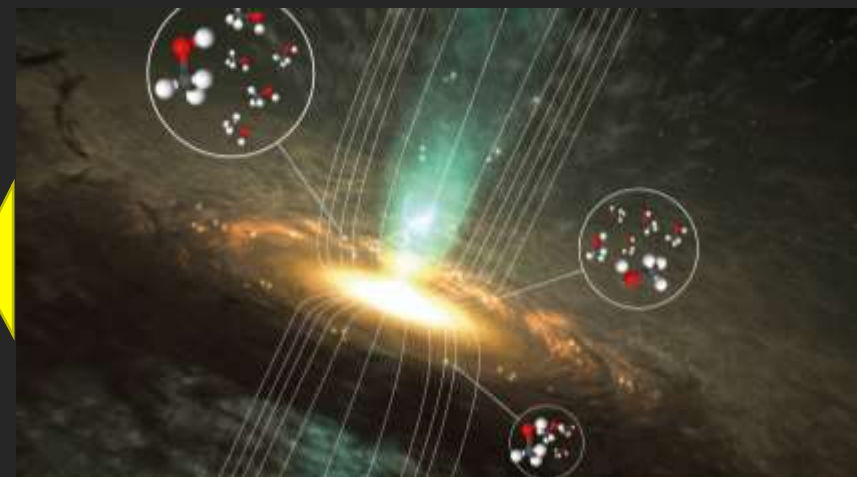
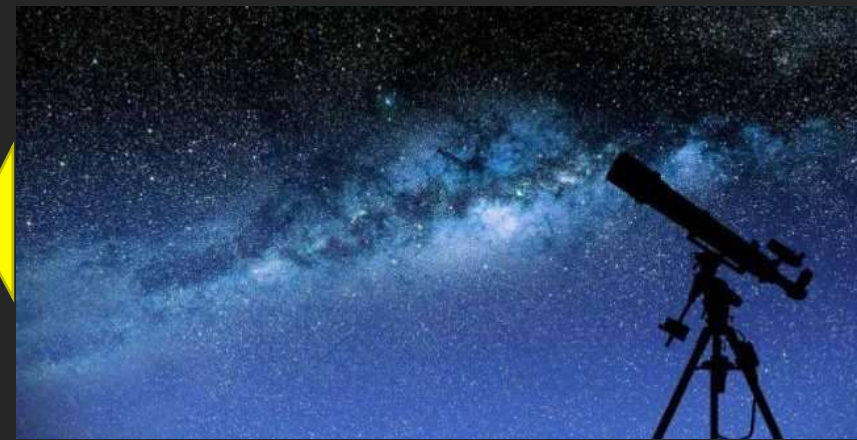


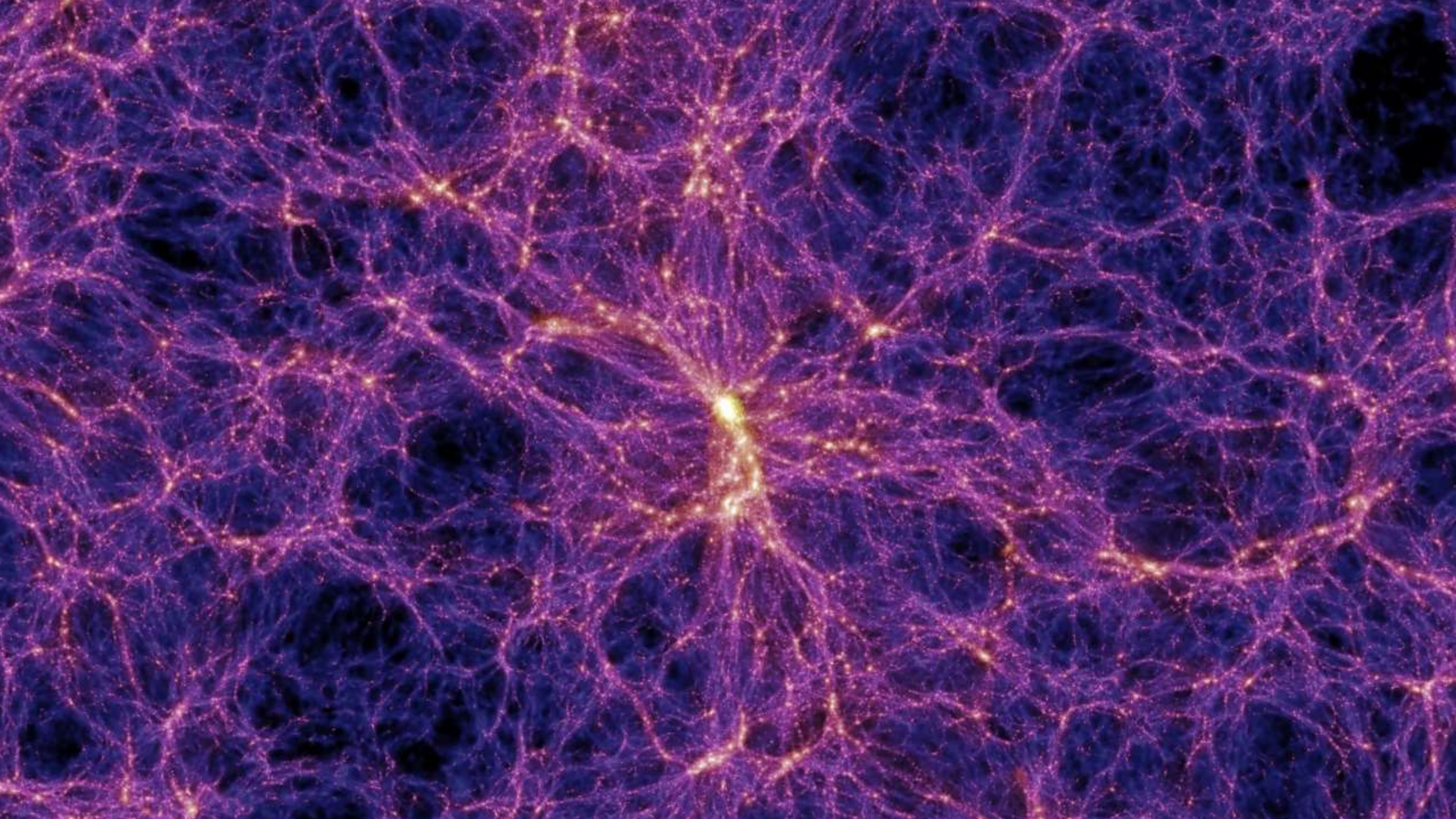


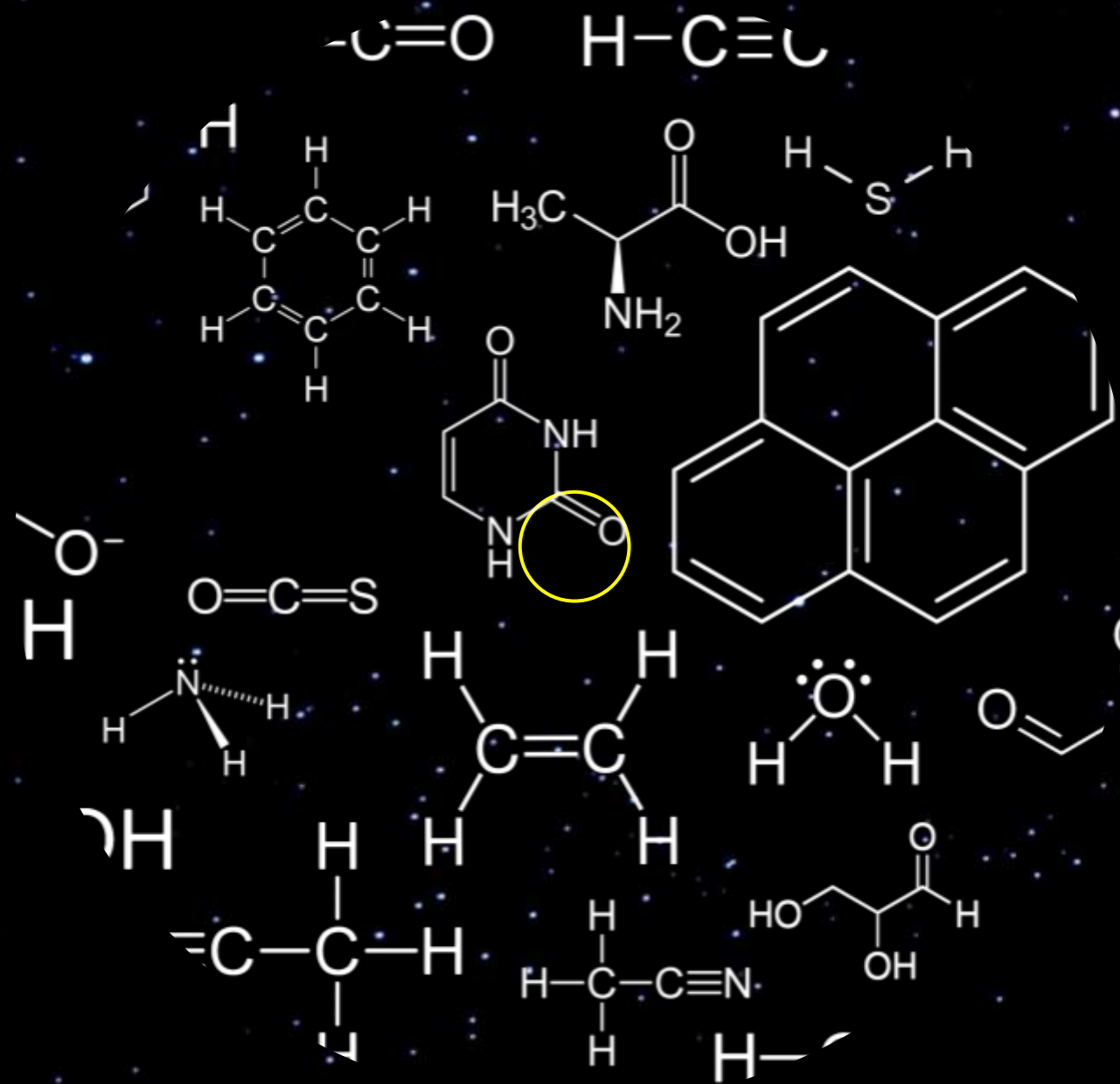
ASTROCHIMICA

CHI, COSA, DOVE, COME, QUANDO, PERCHÉ





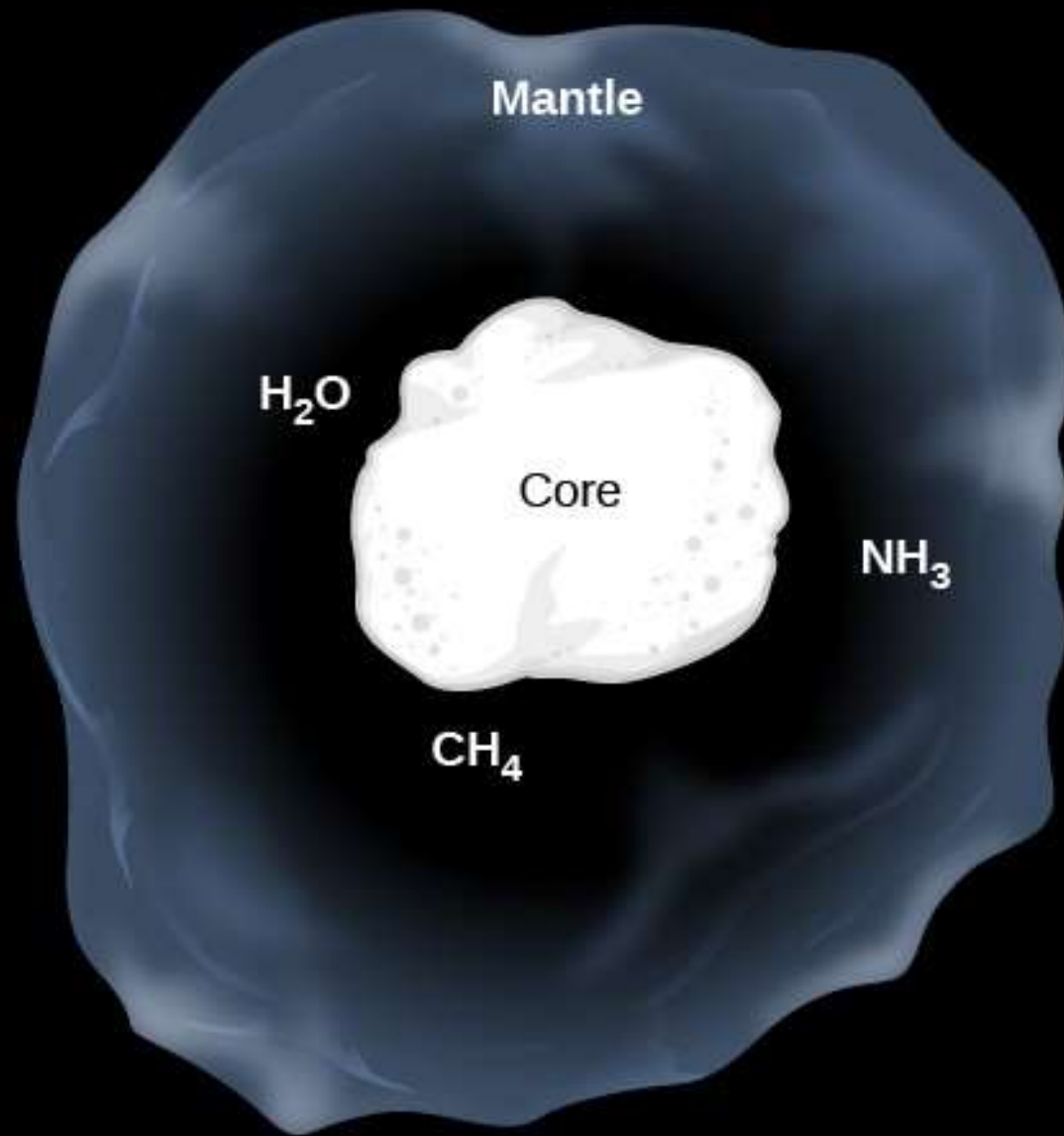




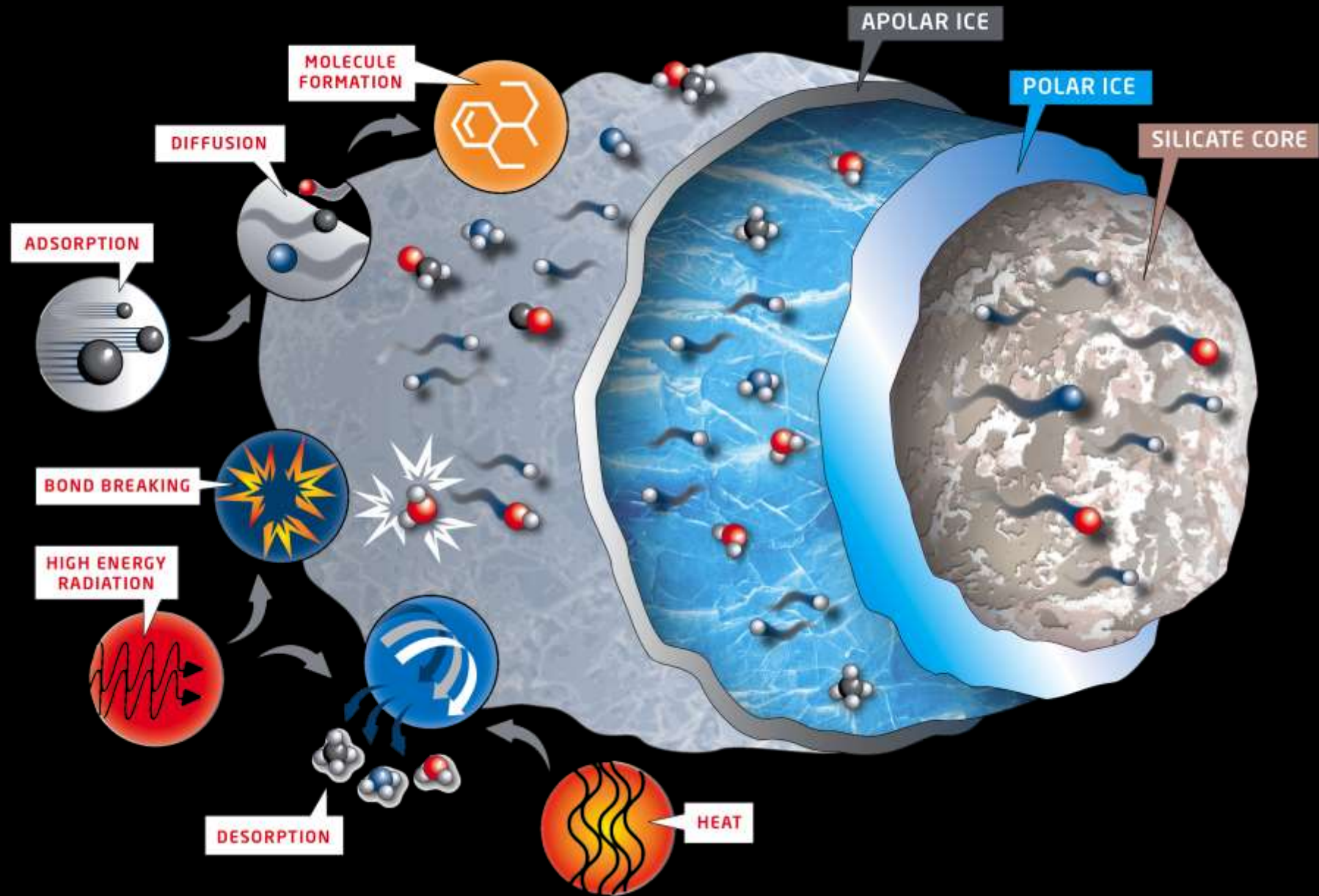
Alcune sostanze
rilevate in
ambienti di
interesse
astrochimico:
comete e medium
interstellare

Table 4 Representative abundances of molecules observed in comets and interstellar sources^a

Molecule	Comets ^b					Interstellar Sources		
	Halley	Hyakutake	Hale-Bopp	2001 A2	73P/SW3	L134N ^c	IRAS 16293 ^d	Sgr B2(N) ^e
CO	3.5–11	14–30	12–23	4	0.5	26,400	8,000	1,000
CO ₂	3–4	...	6	...	...	...	...	...
CH ₄	<0.8	0.8	1.5	1.2	< 0.25	...	...	...
C ₂ H ₂	0.3	0.2–0.5	0.1–0.3	0.5	<0.04	...	...	...
C ₂ H ₆	0.4	0.6	0.6	1.7	0.14	...	...	...
CH ₃ OH	1.8	2	2.4	2.8–3.9	0.22	1	10	3–200
H ₂ CO	4	1	1.1	0.24	0.14	6.6	2	0.5
HCOOH	...	...	0.09	...	...	0.1	<0.03	0.1
HCOOCH ₃	...	...	0.08	...	...	...	0.09	1
CH ₃ CHO	...	...	0.02	...	...	0.2	<0.07	0.2
(CH ₂ OH) ₂	...	...	0.25	...	...	...	...	0.1
CH ₃ OCH ₃	...	...	<0.5	...	...	...	0.16	0.3
NH ₂ CHO	...	...	0.015	...	...	...	<0.001	0.2
NH ₃	1.5	0.5	0.7	...	<0.3	0.08	6	...
HCN	0.1	0.1–0.2	0.25	0.1–0.6	0.25	1.3	0.2	0.4
HNCO	...	0.07	0.1	...	...	...	0.3	0.6
HNC	...	0.01	0.04	0.0066	<0.0013	2.0	0.01	0.1
CH ₃ CN	...	0.01	0.02	0.028	0.030	...	0.25	30
HC ₃ N	...	...	0.02	...	...	0.06	0.03	5
H ₂ S	0.4	0.8	1.5	1.15	0.25	0.3	3	...
CS	...	0.1	0.1	0.07	0.11	0.3	0.6	...
OCS	...	0.1	0.4	...	...	0.7	8	2
SO	...	...	0.3	...	...	6.6	8	...
SO ₂	...	...	0.2	...	...	0.1	3	30
CS ₂	0.2	0.1	0.2	...	...	...	...	...
H ₂ CS	...	...	0.02	...	...	0.2	0.02	20
NS	...	...	0.02	...	...	...	0.02	...
S ₂	...	0.005	...	...	...	...	...	...



interstellar grain surface chemistry



STRUMENTI DELL'ASTROCHIMICA



SPETTROSCOPIA



HPC

APPROCCI METODOLOGICI



TEORICO

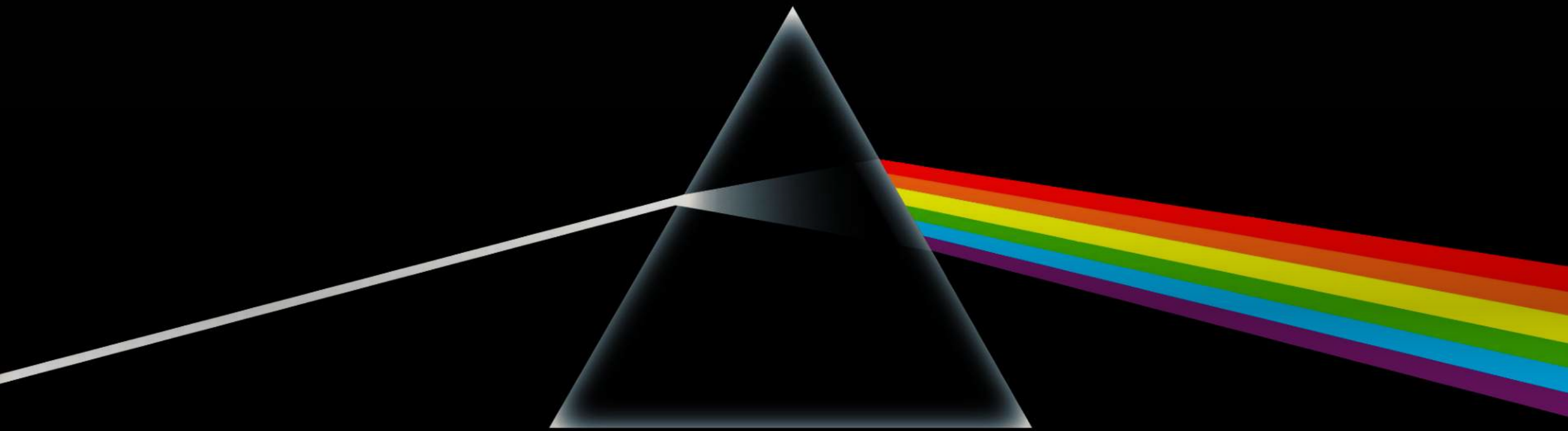


SPERIMENTALE

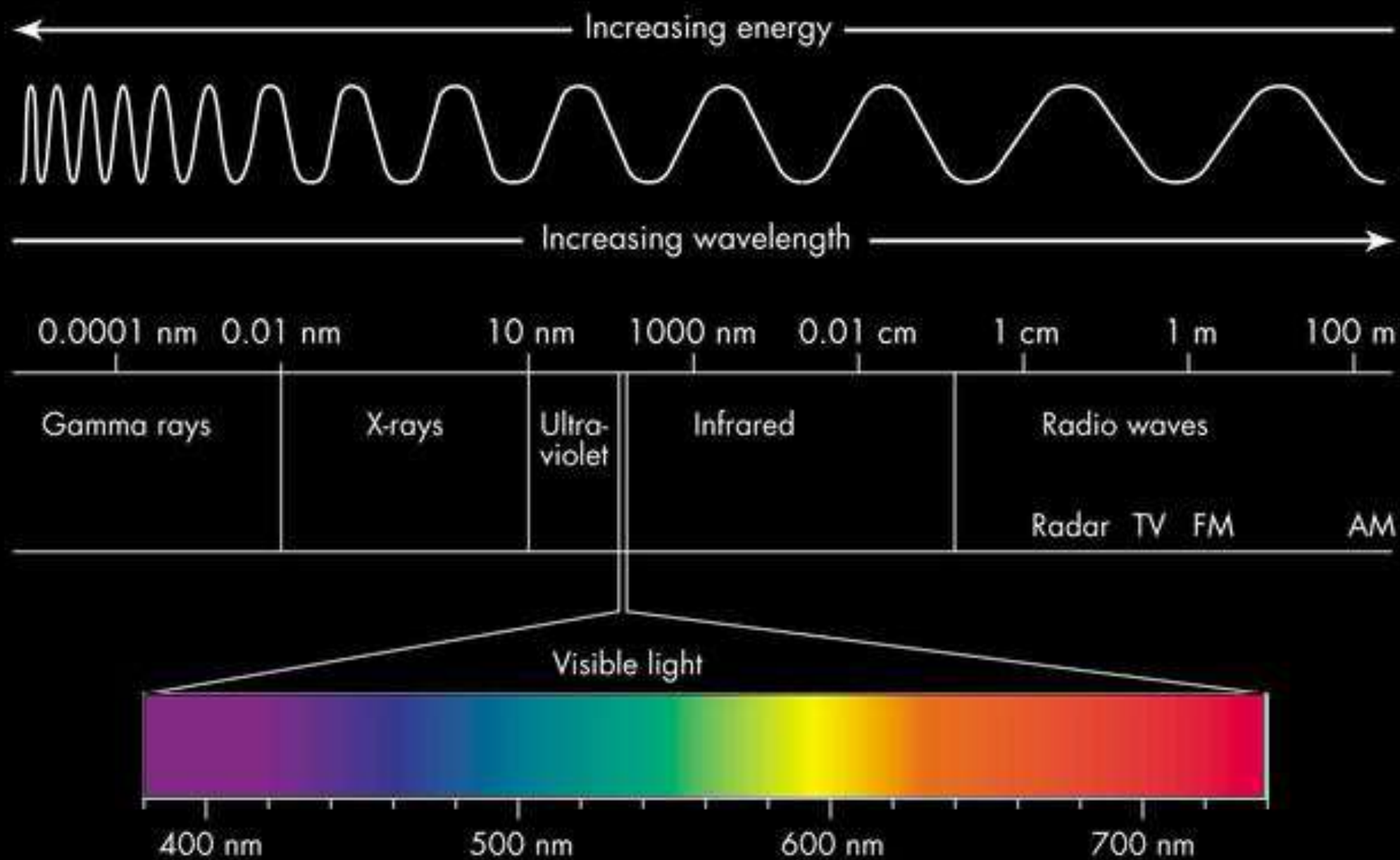


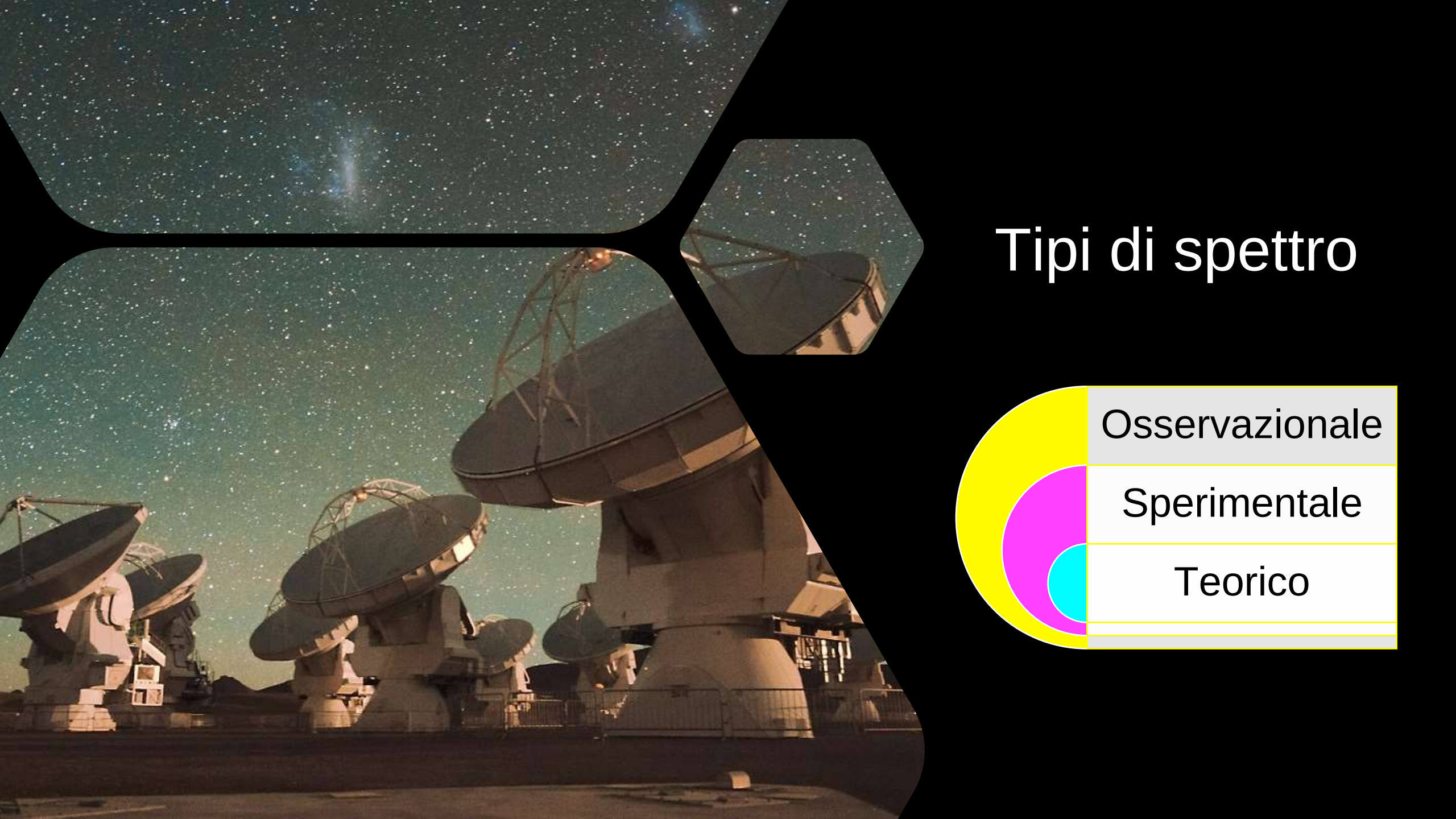
SVILUPPO

SPECTROSCOPY

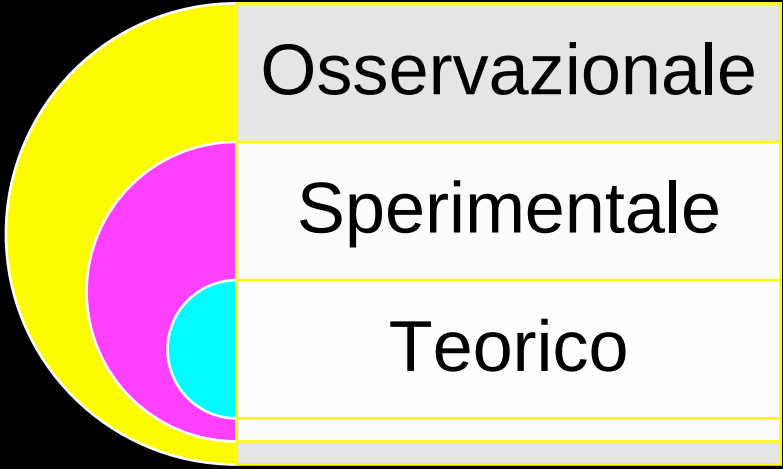


THE DARK SIDE OF THE CHEMISTRY





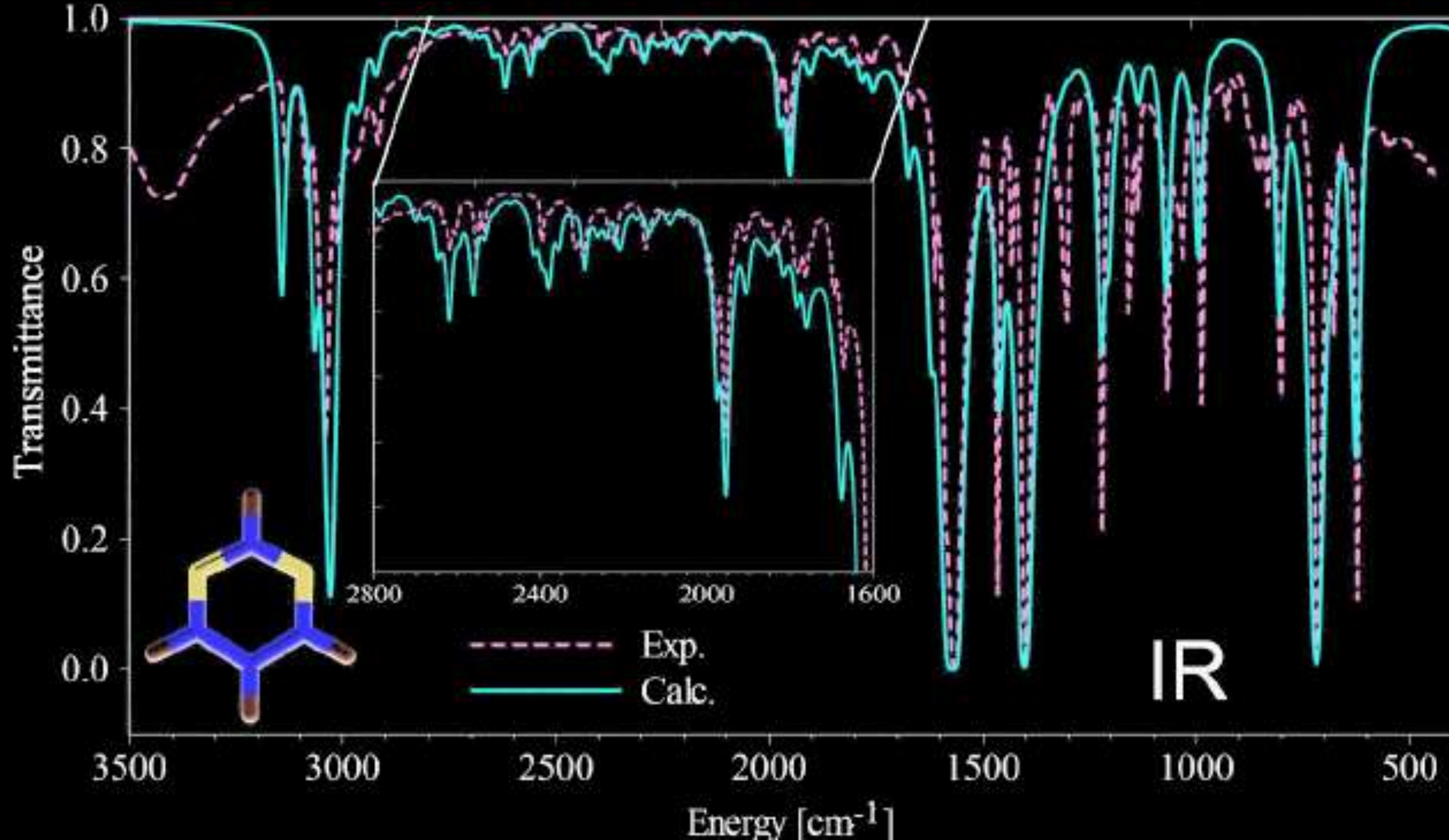
Tipi di spettro

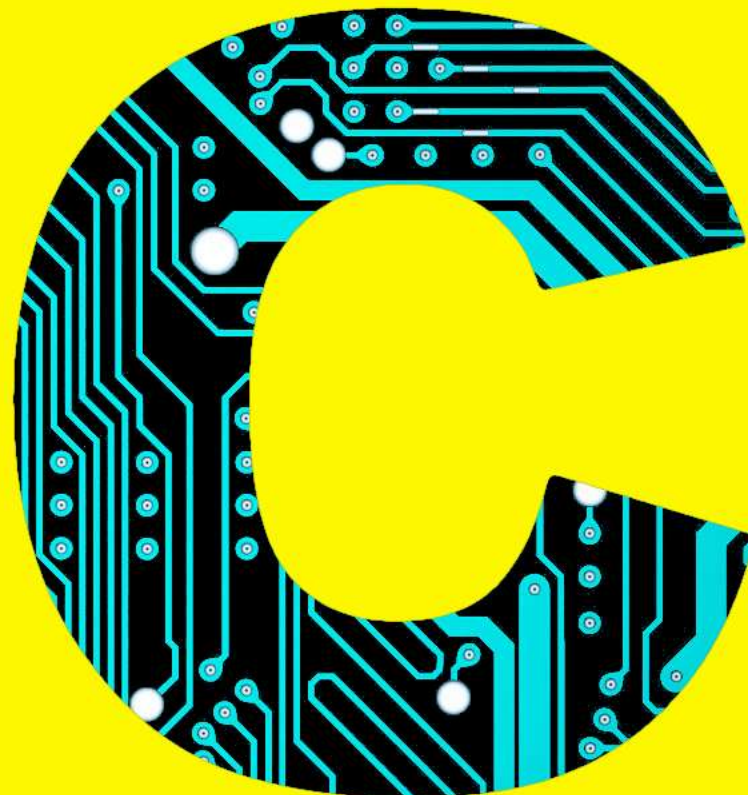
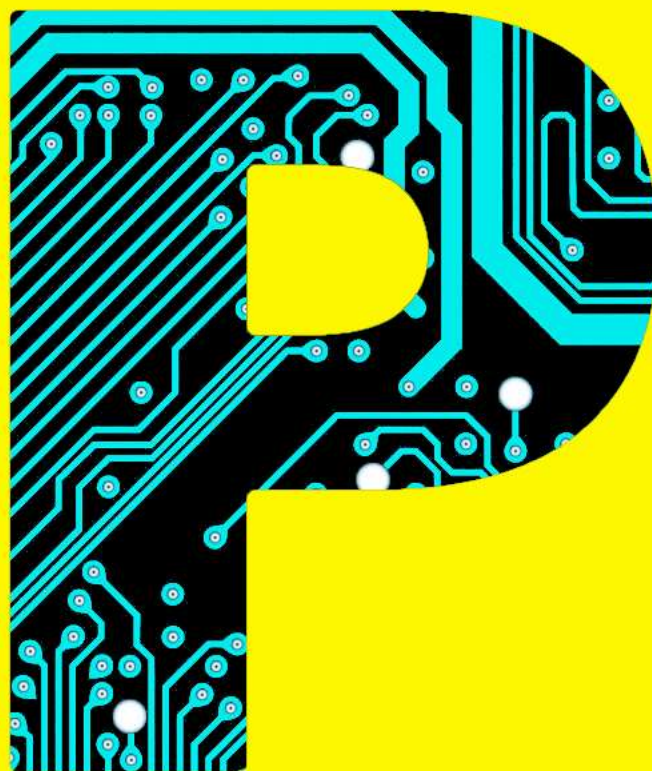
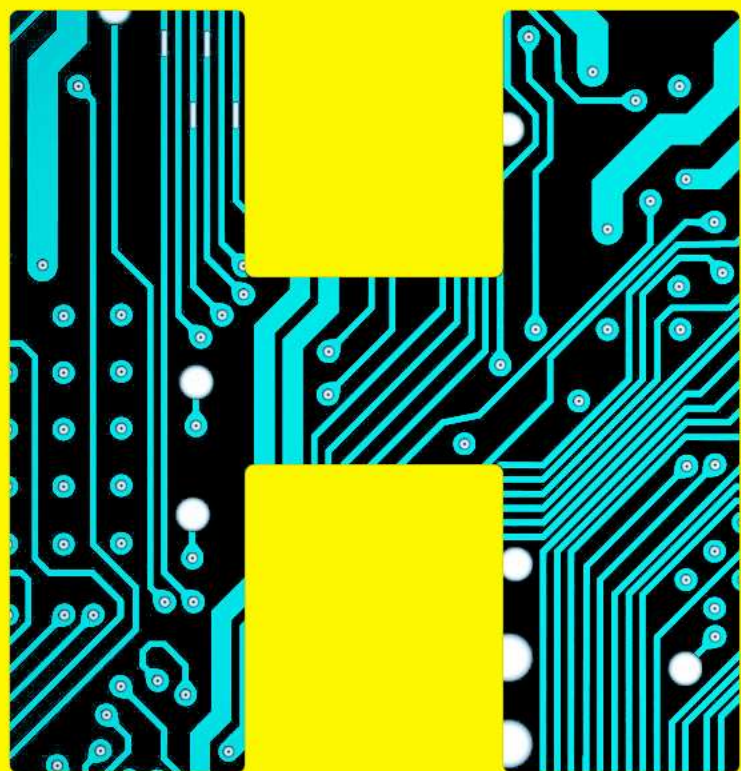


Osservazionale

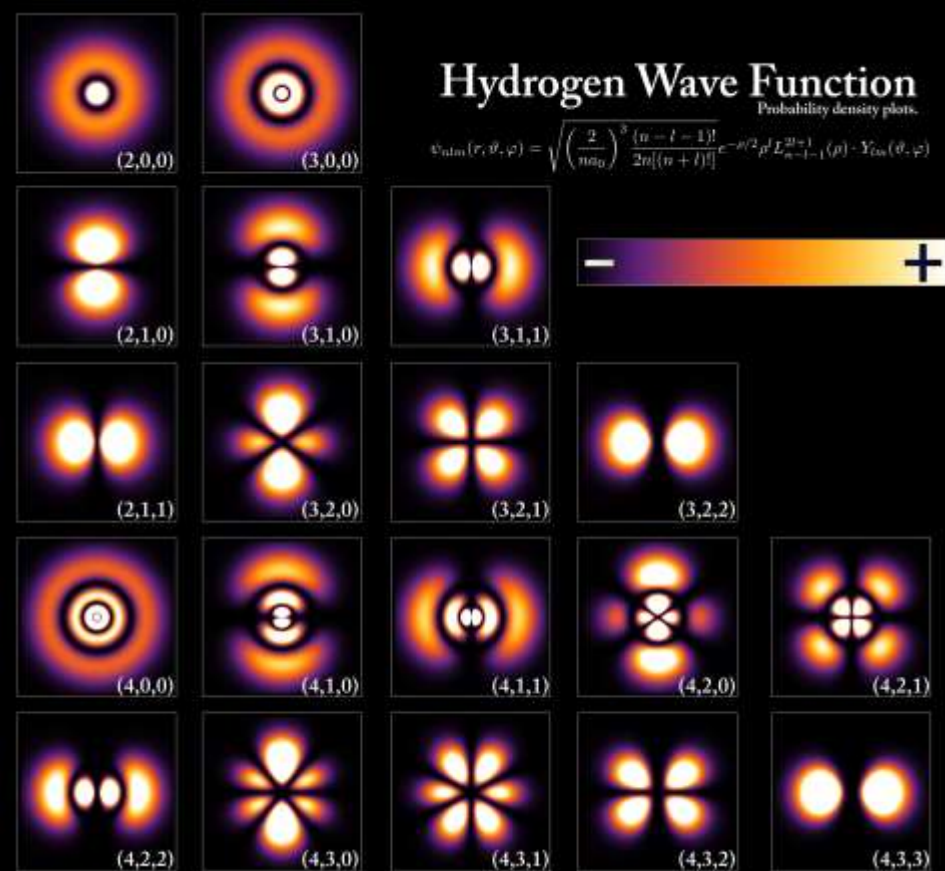
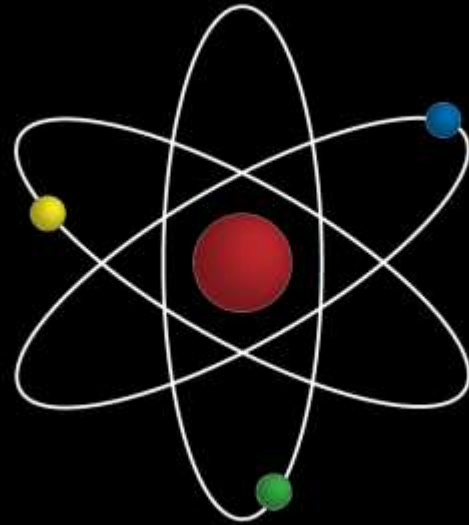
Sperimentale

Teorico





Cluster Name	Total Nodes	Cores per Node	RAM per Node	Notes
Cannizzaro	5	64, 24 or 16 (see notes)	64 or 128 GB (see notes)	The cluster is made by AMD and Intel servers with different number of cores and RAM amount. The nodes also hosts various models of Nvidia GPU cards for CUDA computations.
Curie	28	16	64 GB	
Hoffmann	24	16	128 GB	
Kohn	4	16	24 GB	
Lee	8	24	128 GB	
Mulliken	1	224	6 TB	HPE Superdome Flex Server with ccNUMA architecture (with Hyper-Threading)
Pauling	1	160	4 TB	SGI Ultraviolet 3000 with ccNUMA architecture
Pople	14	64	128 GB	
Vanthoff	1	240	6 TB	SGI Ultraviolet 2000 with ccNUMA architecture
Zewail	6	8	12 GB	



$$\Psi(1, 2, \dots, N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_1(1) & u_2(1) & \cdots & u_N(1) \\ u_1(2) & u_2(2) & \cdots & u_N(2) \\ \vdots & \vdots & \ddots & \vdots \\ u_1(N) & u_2(N) & \cdots & u_N(N) \end{vmatrix}$$

$$H\Psi = E\Psi$$

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{2N}\nabla_i^2 - \sum_{i=1}^{2N}\sum_{A=1}^M\frac{Z_A}{r_{iA}} + \sum_{i=1}^{2N}\sum_{j>i}^{2N}\frac{1}{r_{ij}} + \sum_A^M\sum_{B<A}^M\frac{Z_A Z_B}{R_{AB}}$$

Tipi di Calcolo

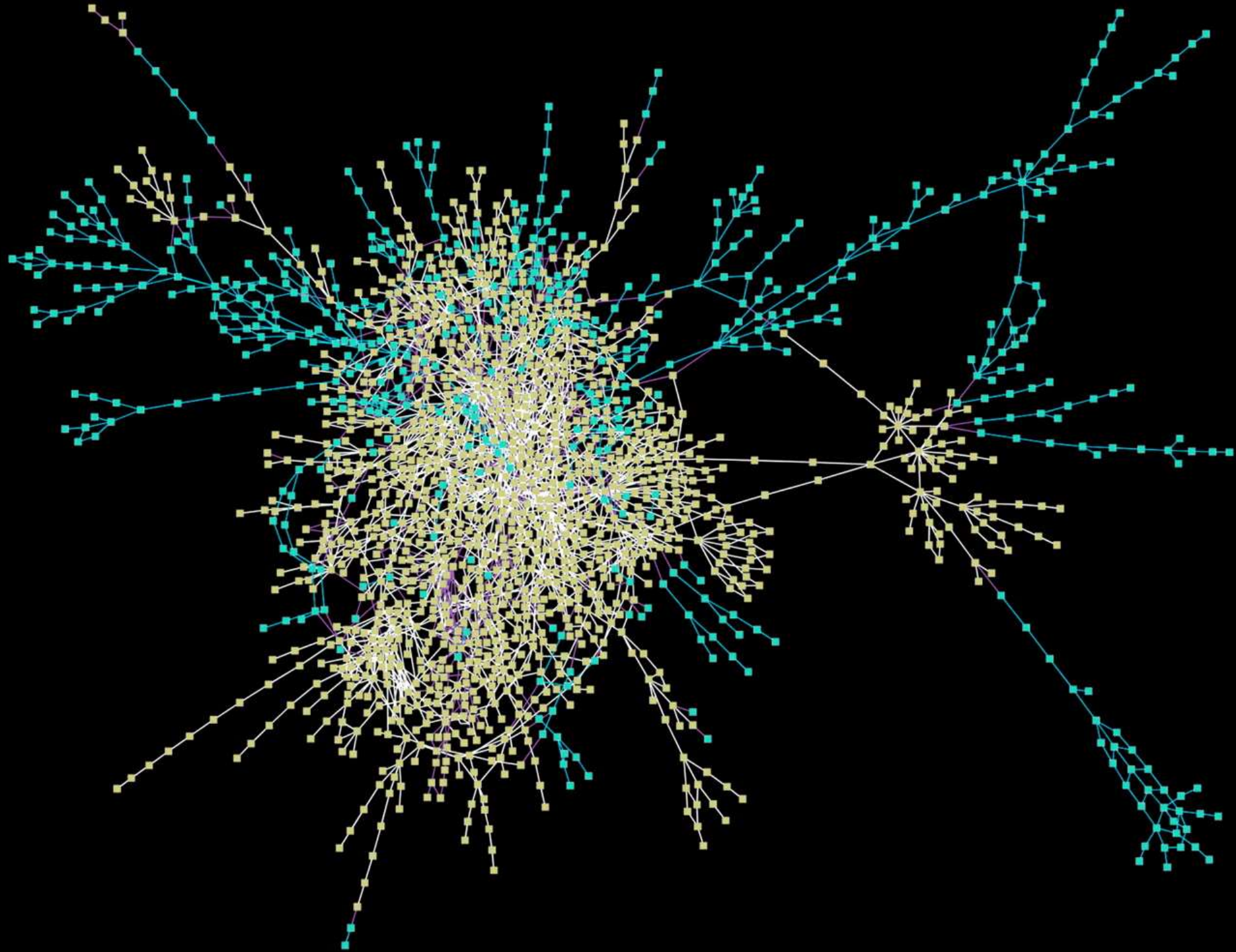
Geometria

Calcolo di spettri

Energia

Reattività





1953



